REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
12-01-2010	Final Report	1-Aug-2005 - 31-Jul-2009

4. TITLE AND SUBTITLE
Final Report: Adaptive Multiscale Analysis of Deposition Processes

5a. CONTRACT NUMBER
W911NF-05-1-0411

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

6. AUTHORS
Mark S. Shephard, Joseph E. Flaherty

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
Rensselaer Polytechnic Institute
Office of Sponsored Research
Rensselaer Polytechnic Institute
Troy, NY 12180 -

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
46359-MA.1

12. DISTRIBUTION AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
Increasingly the models used for many problems of importance must address phenomena occurring on space and time scales ranging over orders of magnitude including electronic, atomic, micro-structural, and system-wide effects. The methods being developed to address these problems face challenging issues including selecting the models for each relevant scale and the coupling information between scales. This project is developing a component-based environment for adaptive multiscale simulation. Our focus is on problems that are modeled by

15. SUBJECT TERMS
multiscale, adaptive, atomistic/continuum

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON / 19b. TELEPHONE NUMBER
UU	UU	UU	UU		Mark Shephard / 518-276-8044

Final Report

Adaptive Multiscale Analysis for Deposition Processes

Proposal Number: 46359MA
Contract Number: W911NF0510411

Professor Mark S. Shephard and Professor Joseph E. Flaherty

Scientific Computation Research Center
Rensselaer Polytechnic Institute
Troy, New York 12180, USA

Statement of Problem Studied

This project addressed two broad objectives. The first was the development of a generalized infrastructure to support the development of adaptive multiscale computational procedures. The second was to develop improved methods to perform atomistic to continuum linkage within the context of concurrent multiscale simulations.

Summary of Most Important Results

The methods and technologies needed to properly couple information across multiple scales represent an active area of research and development. Considering the effort that has gone into the development of the existing single scale simulation tools, a multi-model approach in which interoperable components that build upon, and extend, the developing scale linking technologies to properly coordinate information between existing and new single scale tools is an attractive approach to the development of multiscale simulations. To be effective the resulting simulations must employ adaptive technologies to select and control the models, the discretization techniques and the scale linking methods over the space/time domain of the problem being solved.

We developed a set of functional procedures to support the key components of the models, domains and fields involved in the process of a multiscale simulation. The procedures support the construction and transformation of the information associated with these components as the simulation progresses from its high-level specification, to the concrete mathematical representations, through their conversion into computational models that produce the computational systems that are ultimately solved using numerical methods.

The interaction of components between scales requires the support of the complex transformations. For example, when atomistic and continuum methods are linked, the field transformations must deal with issues such as relating quantities with different definitions like atomistic forces and continuum stresses, defining quantities not defined on the fine scale (e.g., temperature), filtering unneeded high-frequency components when moving up in scale, and accounting for statistical variation when traversing scales. In the context of concurrent multiscale methods, these transformations are most effectively

handled through properly defined overalap regions where the different scale models interact.

The model hierarchy implemented in this work consists of three models. The finest is an atomistic model based on the embedded atom method (EAM) potential. A nonlinear elastic continuum model, whose constitutive relation has terms up to third order elastic constants, is the next coarser scale model in the hierarchy. A linear elastic continuum model is the coarsest model in the hierarchy. This combination of models is selected to allow the study of defect nucleation and their defect interactions as they grow. Material behavior is elastic in the absence of dislocation nucleation and motion. The homogeneous elastic deformation behavior of materials prior to the nucleation of defects can be closely captured by the nonlinear and linear elastic continuum models. Third order elastic constants are essential for a proper treatment of finite deformation of crystals and is adaptively applied in the required portions of the domain. The atomistic model is selected for the sub-domains where defects are nucleating and interacting with each other.

Concurrent atomistic to continuum scaling linkage is based on a weak form of the equilibrium equations over the entire problem domain along with boundary conditions and a set of constraint equations over the overlapping region. The weak form is general in the sense that it can be formulated over the domains in an appropriate form at each of the scales, thus supporting, for example, a direct combination of continuum PDE and discrete atomistic models.

Two error indicators were defined to facilitate the adaptive selection of models from the model hierarchy. The relative error in the energy computed by the two continuum models over an element of a finite element discretization is used as an indicator to select between the nonlinear model and the linear model. A combined criterion is used to detect instability in the continuum model and predict possible dislocation nucleation thus indicating the need for an atomistic model. The first component is an instability bifurcation criterion based on the magnitude of local stress and the second is a stress gradient-based defect nucleation criterion.

The concurrent multiscale simulation process incorporates the indicators to adaptively select different computational models from the model hierarchy and assign them to different sub-domains of the problem domain. The procedure is used in an automated system in which the linear limit is found based on a first continuum level analysis. From that point incremental load steps are applied. At each load step the boundaries between different computational models are adjusted according to the error indicators. An in-house finite element procedure is used to discretize the continuum models and the atomistic regions are solved with either an in-house atomisitic code or the LAMMPS molecular dynamics code from Sandia.

Key accomplishments in the development of a generalized infrastructure to support the development of adaptive multiscale computational procedures include:

- A proper decomposition of a simulation into the four levels of a general problem statement, mathematical representation, computational representation and

numerical system in which the three key informational components of domains, models and fields are transformed from one level to the next through transformations processes and where, in multiscale simulations, the informational components on each level are related by the appropriate transformations between the models on the different scales.
- Construction of a multiscale computational infrastructure that can support the adaptive control of the approximations introduced by each of the transformation processes executed.
- The application of the resulting infrastructure to construct both hierarchic and concurrent multiscale adaptive simulation procedures.

Key accomplishments in the development of atomistic to continuum scale linking methods include:

- A new approach to a zero temperature scale linkage based on a combined atomistic and continuum variational statement, generalized constraints and overlap region blend.
- Adaptive control of the application of atomistic models based on the potential onset of dislocation formation that the continuum models could not represent.
- A finite temperature atomistic to continuum scale linking method (developed by Professor Picu under ARL SBIR and STTR funds).